

10/923,271

<http://www.cas.org/legal/infopolicy.html>

=> file casreact		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
FULL ESTIMATED COST	ENTRY	SESSION
	0.48	0.69

FILE 'CASREACT' ENTERED AT 14:13:04 ON 16 JUN 2008
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FILE CONTENT:1840 - 14 Jun 2008 VOL 148 ISS 25

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* *

Some CASREACT records are derived from the ZIC/VINITI database (1974-1999) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

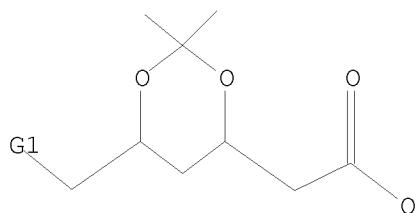
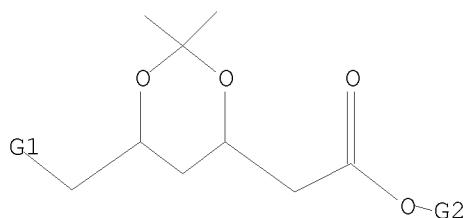
This file contains CAS Registry Numbers for easy and accurate substance identification.

=>
Uploading C:\Program Files\Stnexp\Queries\164.str

L1 STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1 STR

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G1 C,CN,OH

G2 H,Cs,Fr,K,Li,Na,Rb

Structure attributes must be viewed using STN Express query preparation.

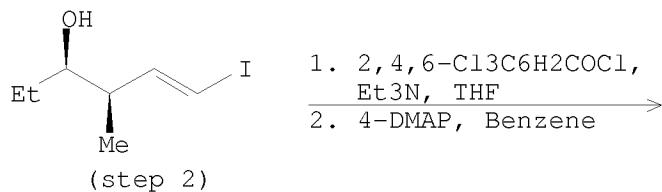
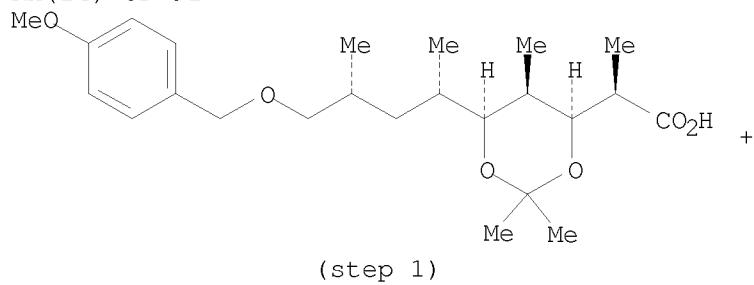
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=> s 11 full
FULL SEARCH INITIATED 14:13:54 FILE 'CASREACT'
SCREENING COMPLETE -      12038 REACTIONS TO VERIFY FROM      461 DOCUMENTS
100.0% DONE    12038 VERIFIED      133 HIT RXNS          23 DOCS
SEARCH TIME: 00.00.02
```

L2 23 SEA SSS FUL L1 (133 REACTIONS)

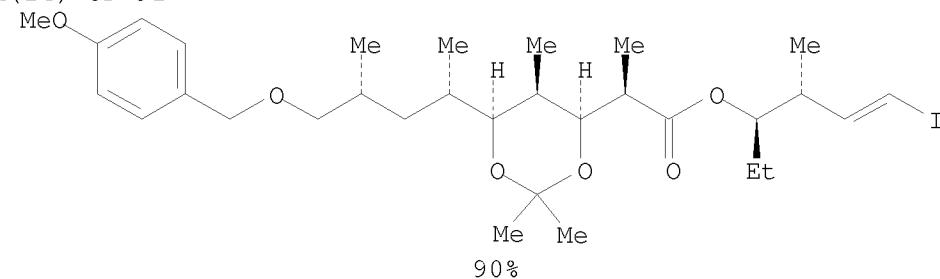
=> d 1-23

L2 ANSWER 1 OF 23 CASREACT COPYRIGHT 2008 ACS on STN

RX(14) OF 91



RX(14) OF 91

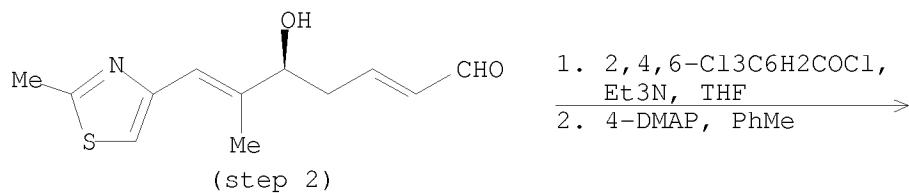
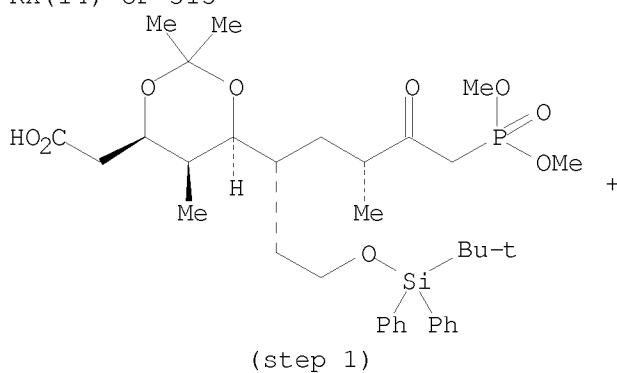


REF: Journal of Organic Chemistry, 70(18), 7267-7272; 2005

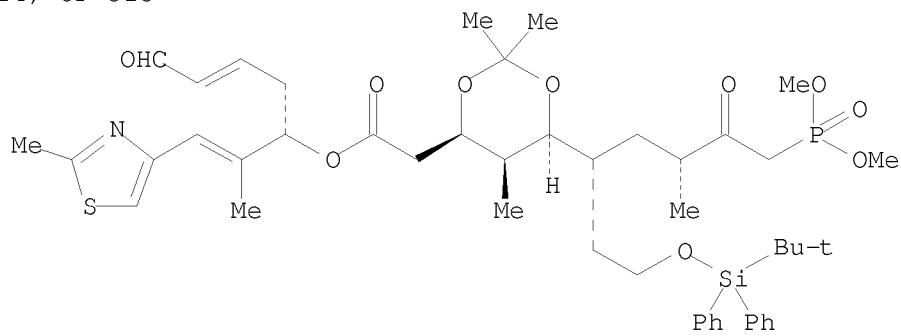
CON: STAGE(1) 2 hours, room temperature

STAGE(2) 24 hours, room temperature

RX(14) OF 315



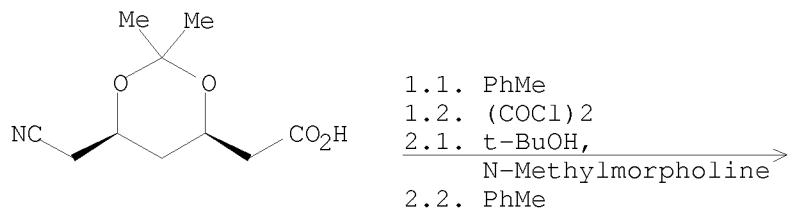
RX(14) OF 315



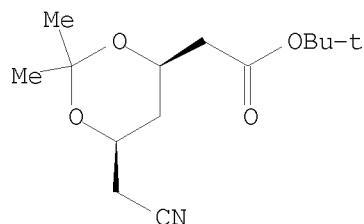
REF: Heterocycles, 64,, 333-345; 2004
 CON: STAGE(1) 1 hour, room temperature
 STAGE(2) 23 hours, room temperature

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RX(11) OF 18 - 2 STEPS



Na



REF: PCT Int. Appl., 2004096788, 11 Nov 2004

NOTE: 1) first stage Dean Stark app.

CON: STEP(1.1) room temperature

STEP(1.2) 2.5 hours, room temperature; 4 hours, room temperature

STEP(2.1) room temperature

STEP(2.2) 30 minutes, room temperature; 12 hours,
room temperature

L2 ANSWER 4 OF 23 CASREACT COPYRIGHT 2008 ACS on STN

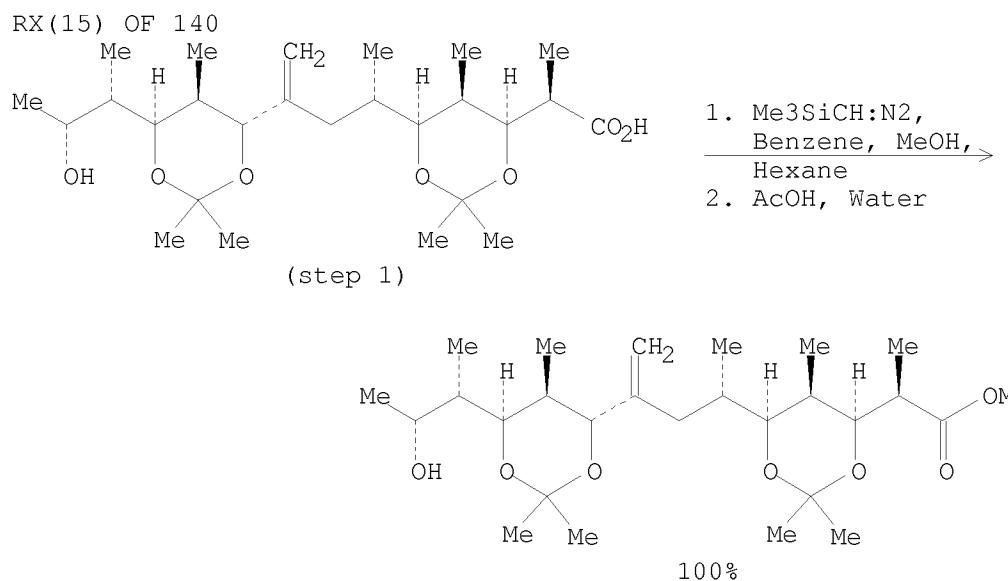
RX(38) OF 521 - REACTION DIAGRAM NOT AVAILABLE

L2 ANSWER 5 OF 23 CASREACT COPYRIGHT 2008 ACS on STN

TOh

16/06/2008

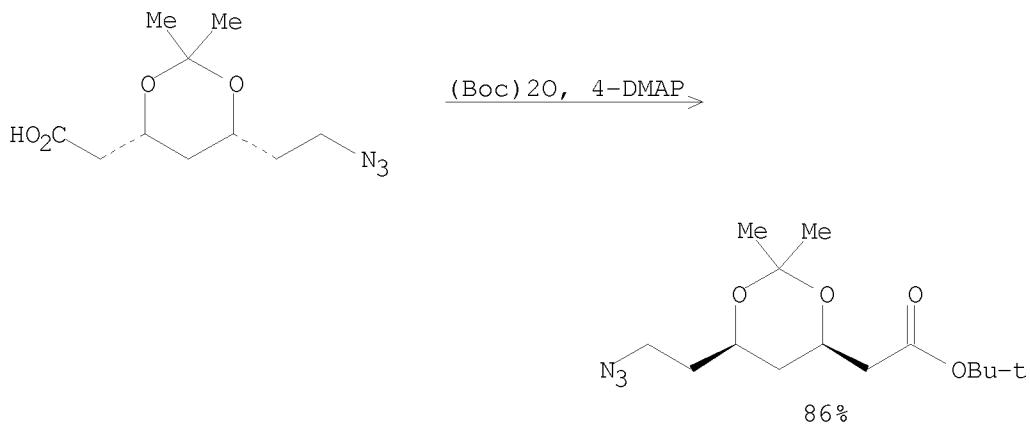
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REF: Tetrahedron, 60(21), 4693-4704; 2004
CON: STAGE(1) 45 minutes, room temperature
STAGE(2) room temperature

L2 ANSWER 6 OF 23 CASREACT COPYRIGHT 2008 ACS on STN

RX(8) OF 43

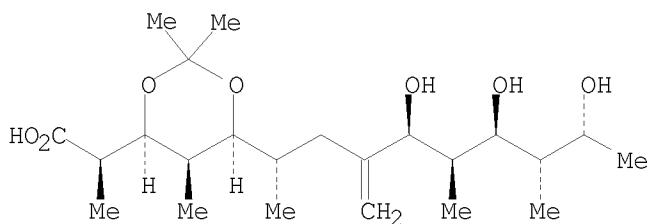
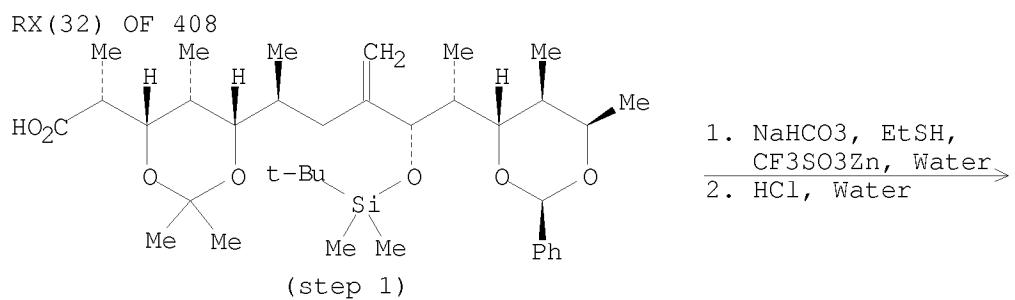


REF: Tetrahedron Letters, 45(11), 2439-2441; 2004

L2 ANSWER 7 OF 23 CASREACT COPYRIGHT 2008 ACS on STN

TOh

16/06/2008



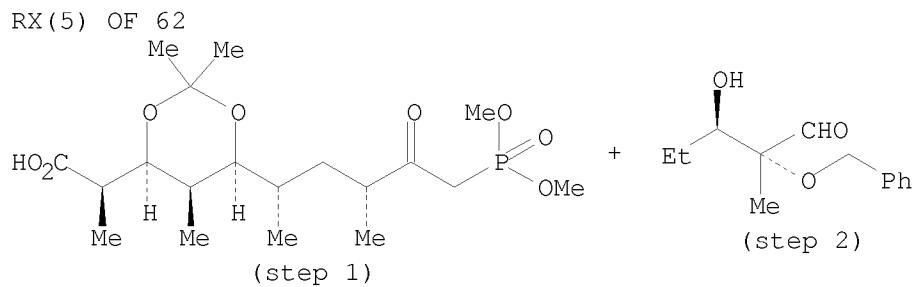
REF: Journal of the American Chemical Society, 124(43), 12806-12815;

2002

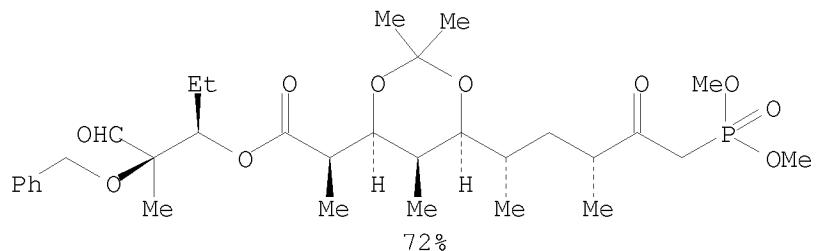
CON: STAGE(1) 2 hours, 0 deg C; 13 hours, room temperature

STAGE(2) pH 4

L2 ANSWER 8 OF 23 CASREACT COPYRIGHT 2008 ACS on STN



1. 4-DMAP, Et3N, PhMe

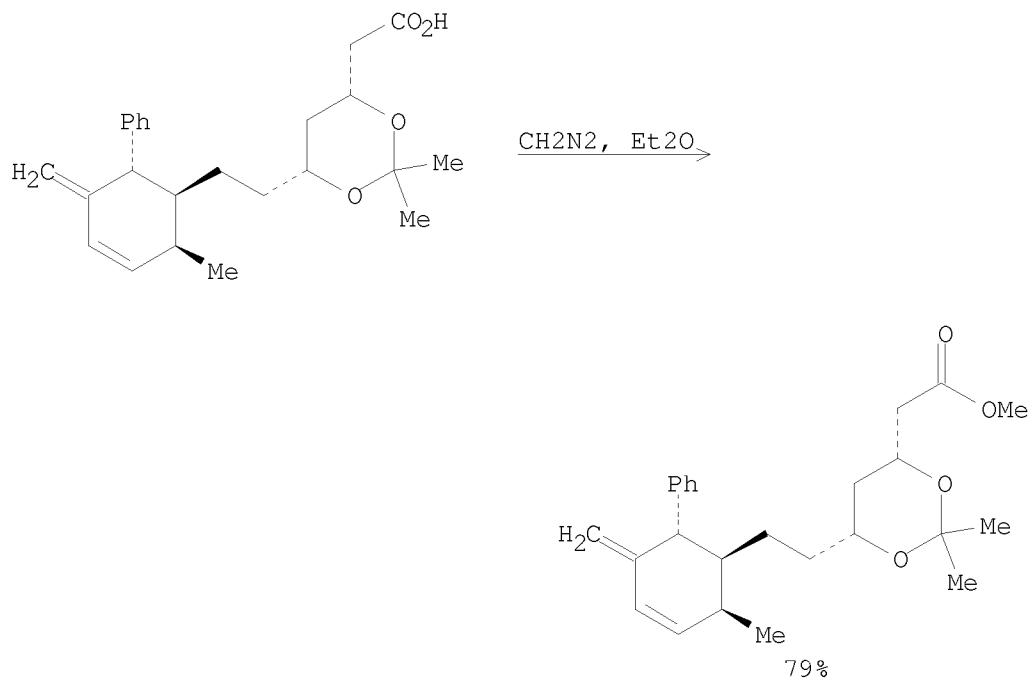


REF: Heterocycles, 46,, 105-110; 1997
 NOTE: key step

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L2 ANSWER 9 OF 23 CASREACT COPYRIGHT 2008 ACS on STN

RX(10) OF 66

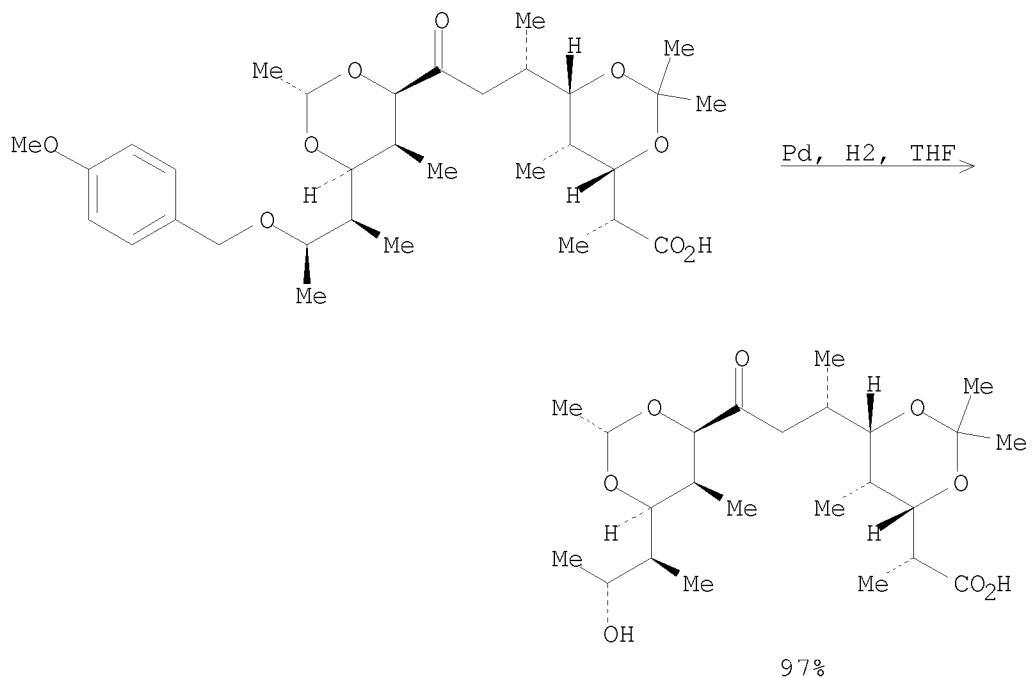


REF: Journal of Organic Chemistry, 60(17), 5532-6; 1995

L2 ANSWER 10 OF 23 CASREACT COPYRIGHT 2008 ACS on STN

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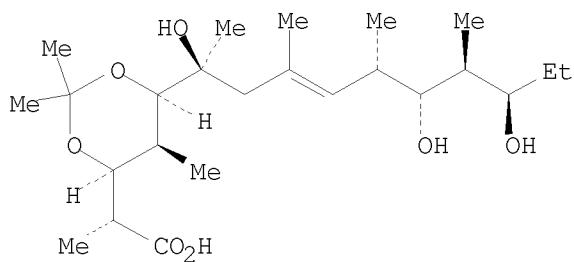
RX(39) OF 654



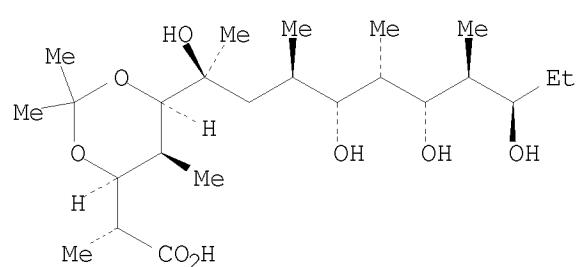
REF: Journal of the American Chemical Society, 116(25), 11287-314;
1994

L2 ANSWER 11 OF 23 CASREACT COPYRIGHT 2008 ACS on STN

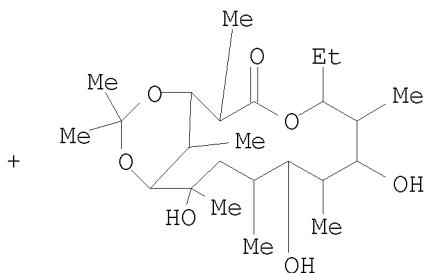
RX(29) OF 229 - 2 STEPS



1.1. Et₃N,
2,4,6-Cl₃C₆H₂COCl,
THF
1.2. 4-DMAP, PhMe
2.1. BH₃-Me₂S, THF
2.2. H₂O₂, NaOH,
Water



13%



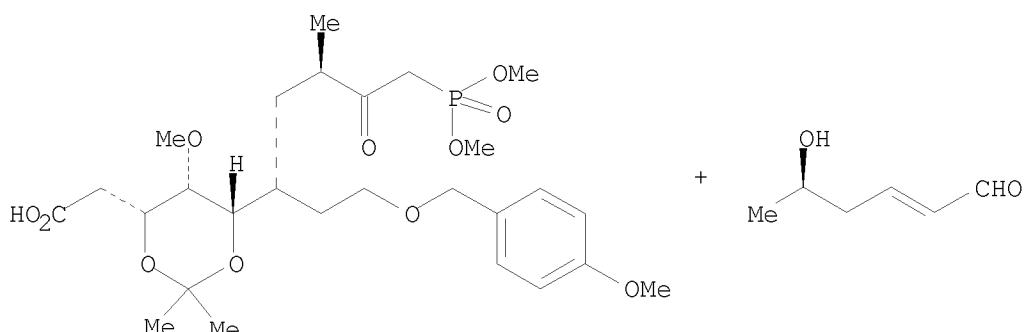
stereoisomers
72%

REF: Journal of the American Chemical Society, 113(3), 910-23; 1991

NOTE: 1) 2nd step thermal

L2 ANSWER 12 OF 23 CASREACT COPYRIGHT 2008 ACS on STN

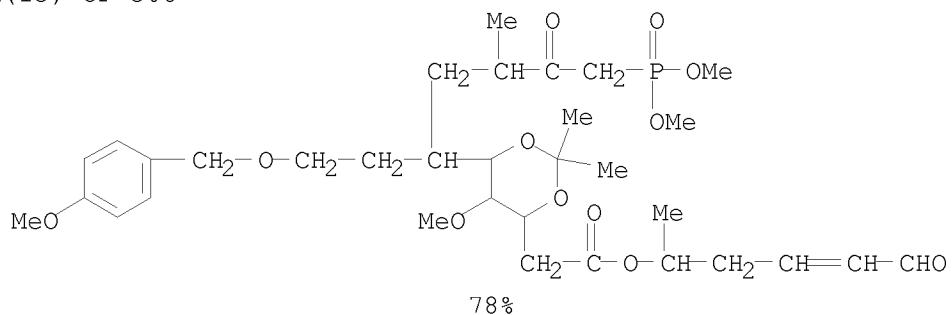
RX(13) OF 306



4-DMAP, R:84033-23-8, →
PhMe

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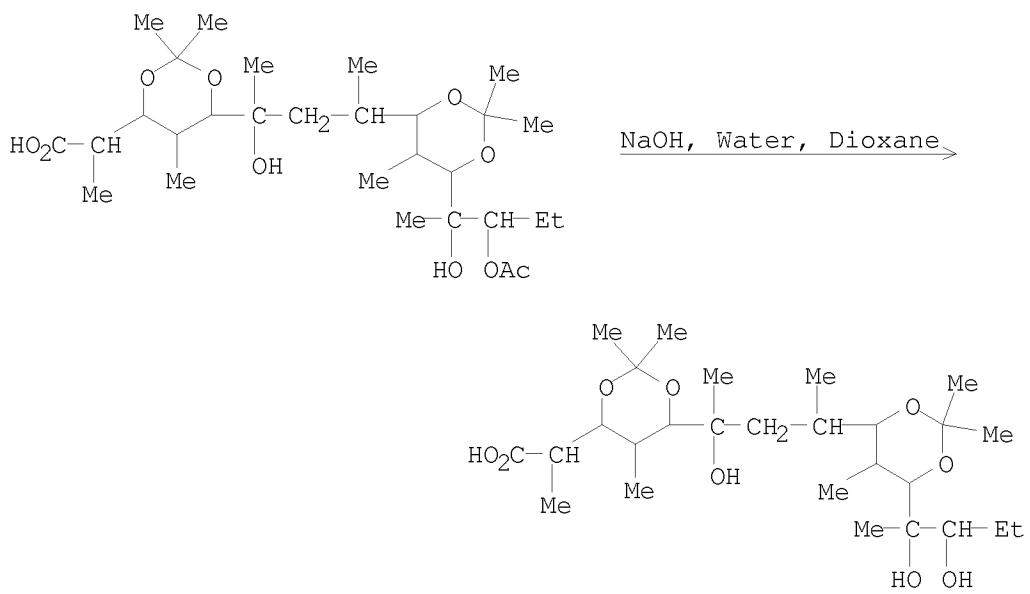
RX(13) OF 306



REF: Heterocycles, 31(1), 5-8; 1990

L2 ANSWER 13 OF 23 CASREACT COPYRIGHT 2008 ACS on STN

RX(65) OF 715

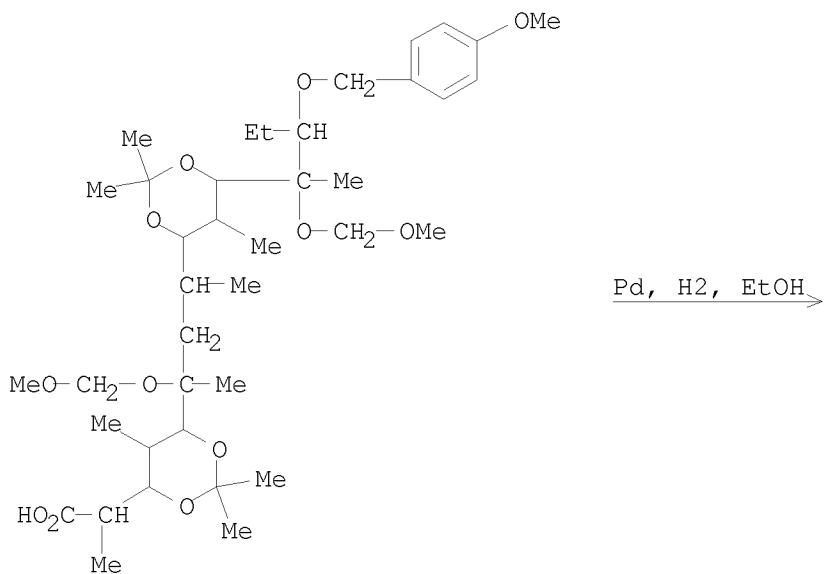


REF: Bulletin of the Chemical Society of Japan, 62(8), 2618-35; 1989

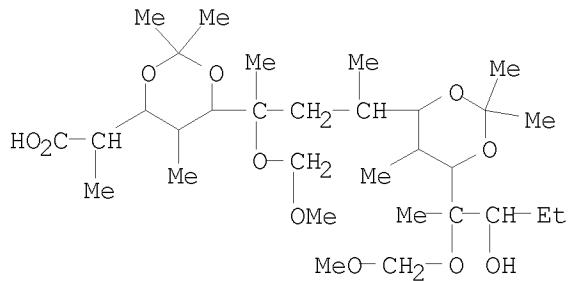
L2 ANSWER 14 OF 23 CASREACT COPYRIGHT 2008 ACS on STN

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RX(18) OF 319



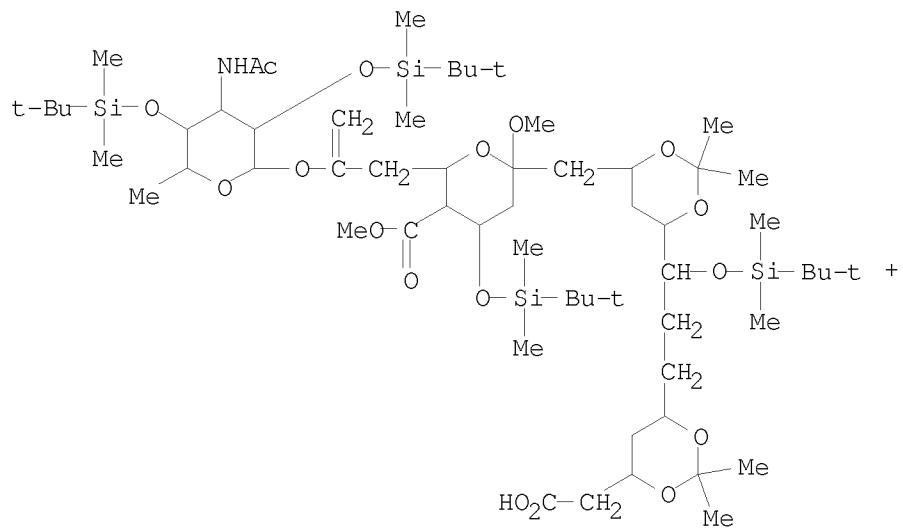
RX(18) OF 319



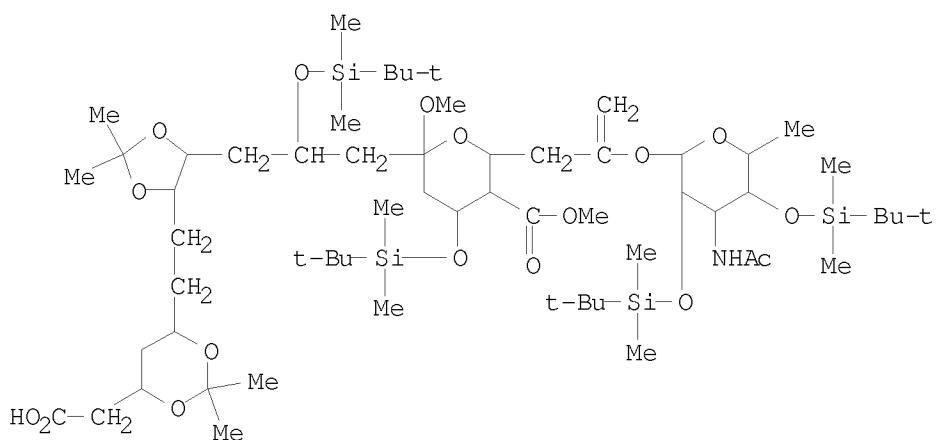
REF: Chemical & Pharmaceutical Bulletin, 37(5), 1167-72; 1989

L2 ANSWER 15 OF 23 CASREACT COPYRIGHT 2008 ACS on STN

RX(10) OF 179

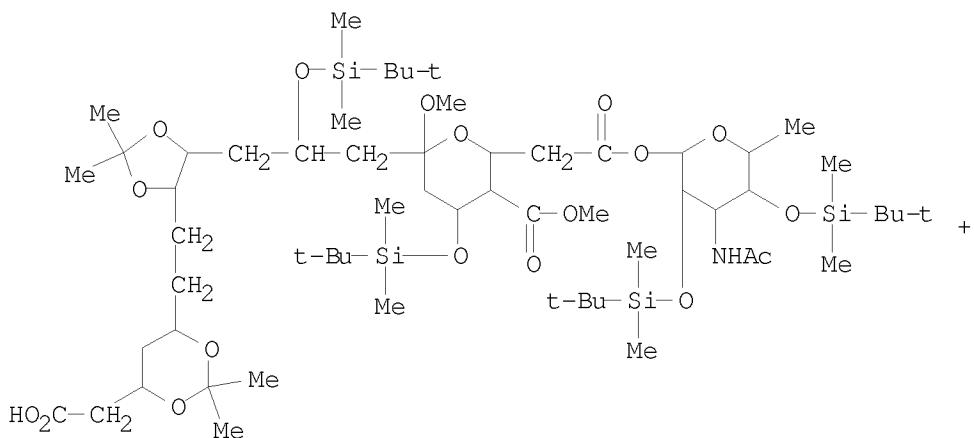


RX(10) OF 179

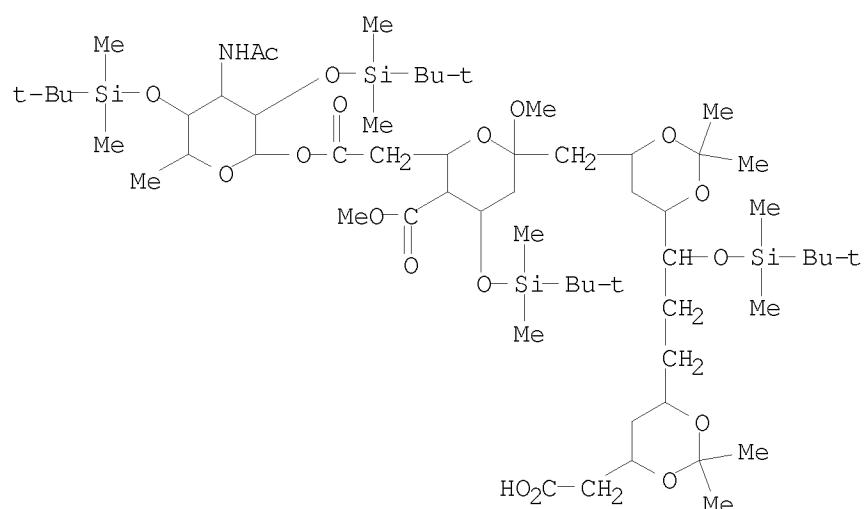
Ozone, MeOH, CH₂Cl₂ →

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RX(10) OF 179



RX(10) OF 179

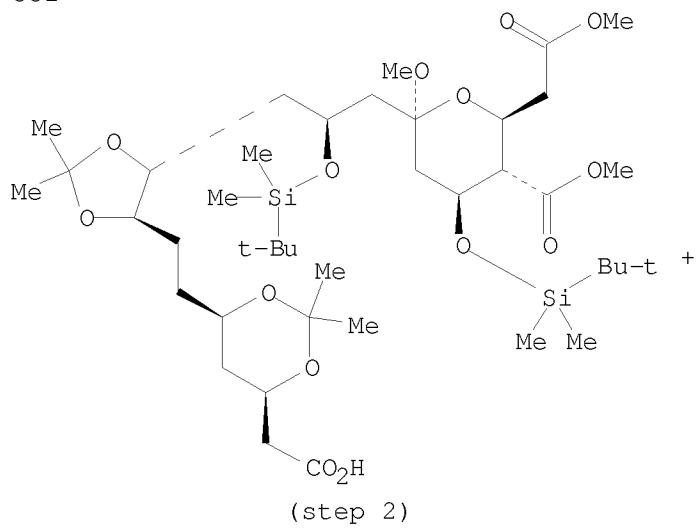


REF: Journal of the American Chemical Society, 110(14), 4660-72;
1988

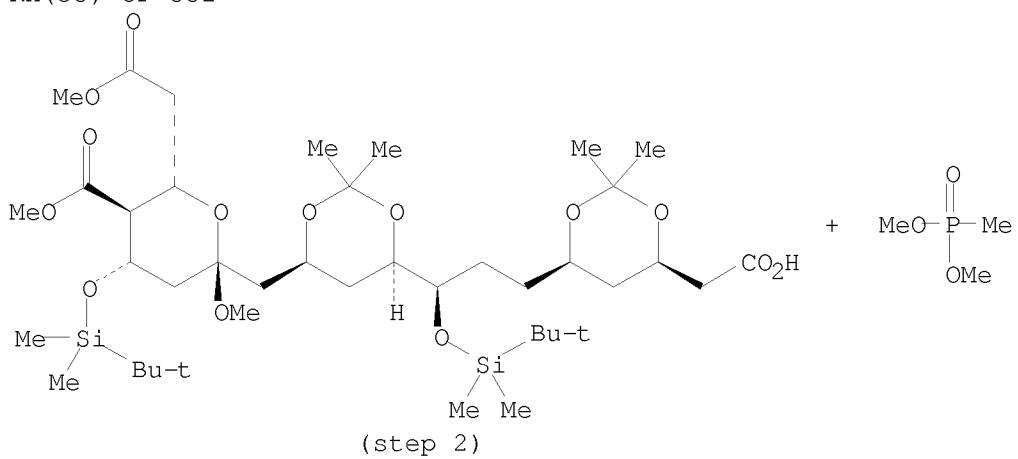
L2 ANSWER 16 OF 23 CASREACT COPYRIGHT 2008 ACS on STN

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RX(35) OF 552



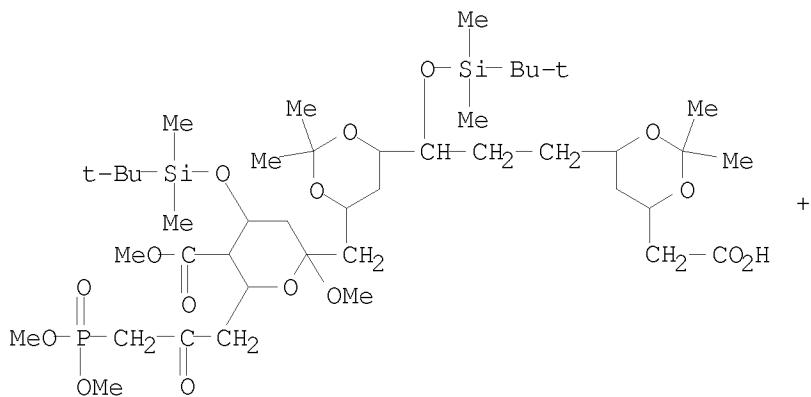
RX(35) OF 552



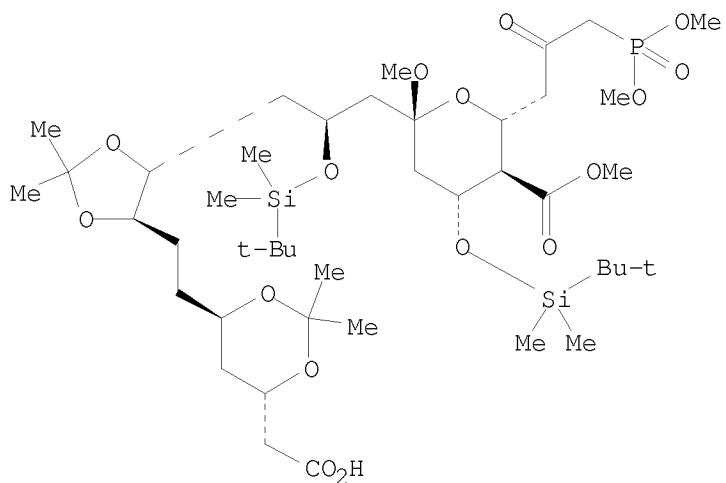
1. BuLi, THF →
2. THF

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RX(35) OF 552



RX(35) OF 552



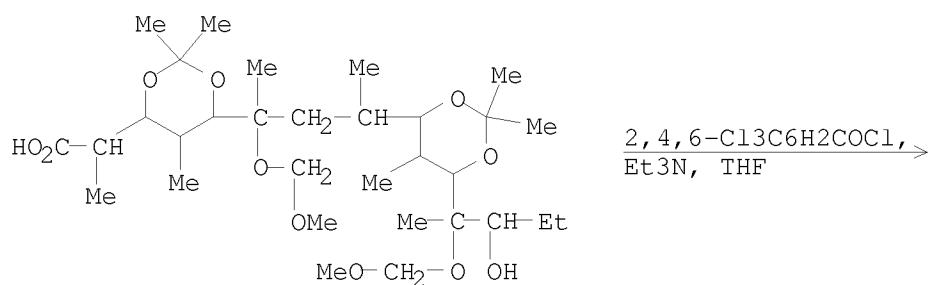
REF: Journal of the American Chemical Society, 110(14), 4685-96;
1988

NOTE: 62% overall

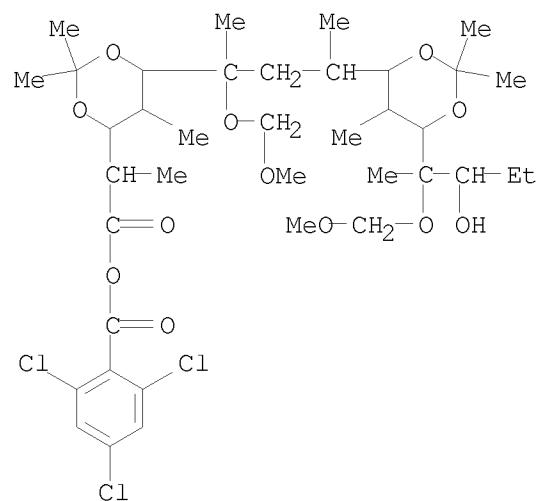
L2 ANSWER 17 OF 23 CASREACT COPYRIGHT 2008 ACS on STN

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RX(32) OF 451



RX(32) OF 451



REF: Tetrahedron Letters, 28(39), 4569-72; 1987

L2 ANSWER 18 OF 23 CASREACT COPYRIGHT 2008 ACS on STN

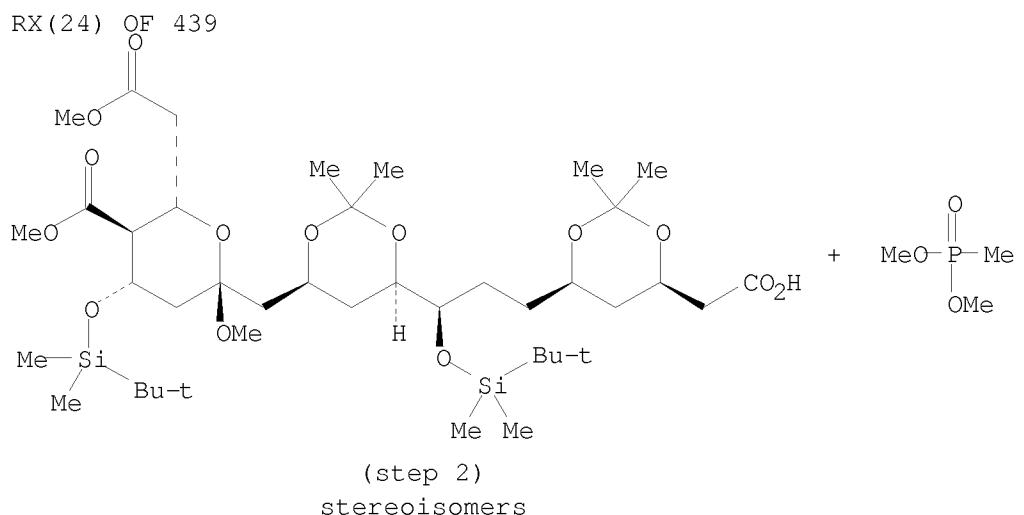
RX(47) OF 265 - REACTION DIAGRAM NOT AVAILABLE

L2 ANSWER 19 OF 23 CASREACT COPYRIGHT 2008 ACS on STN

RX(17) OF 258 - REACTION DIAGRAM NOT AVAILABLE

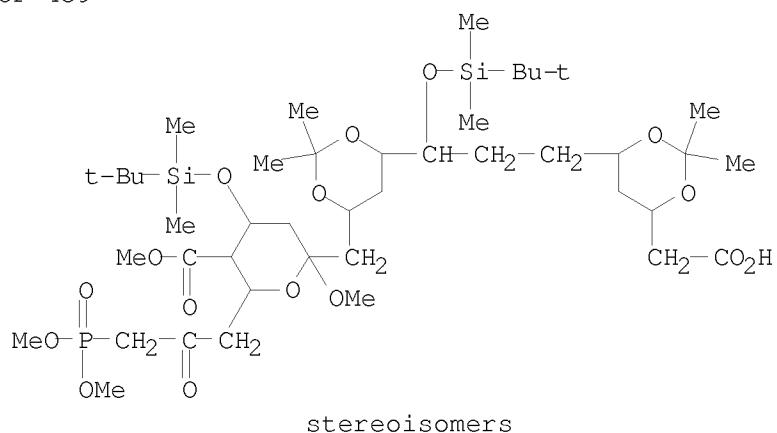
L2 ANSWER 20 OF 23 CASREACT COPYRIGHT 2008 ACS on STN

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1. BuLi, THF →

RX(24) OF 439



REF: Journal of the American Chemical Society, 109(7), 2208-10; 1987
NOTE: 62% OVERALL

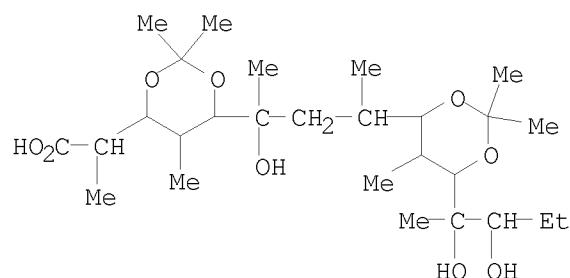
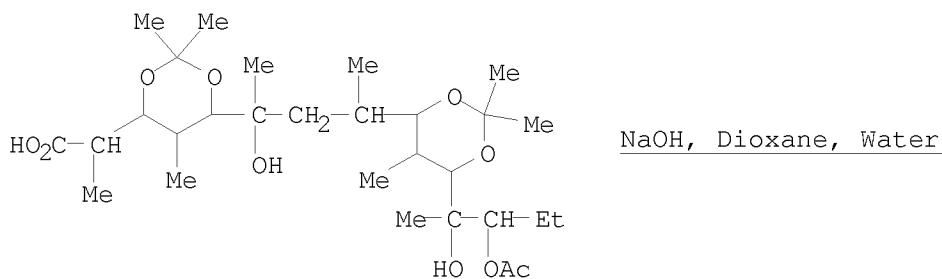
L2 ANSWER 21 OF 23 CASREACT COPYRIGHT 2008 ACS on STN

TOh

16/06/2008

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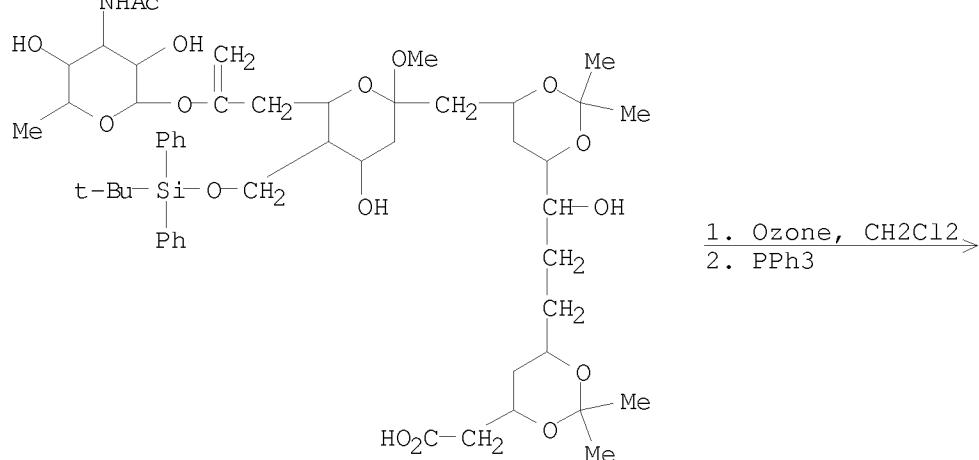
RX(18) OF 316



REF: Tetrahedron Letters, 27(16), 1815-18; 1986

L2 ANSWER 22 OF 23 CASREACT COPYRIGHT 2008 ACS on STN

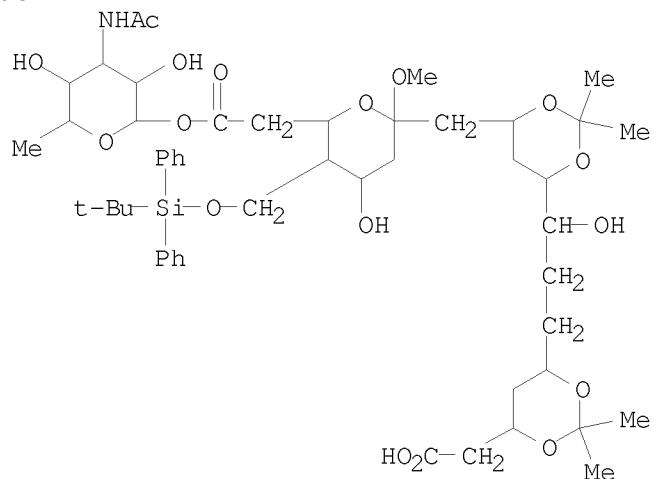
RX(12) OF 395



(step 1)
stereoisomers

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RX(12) OF 395

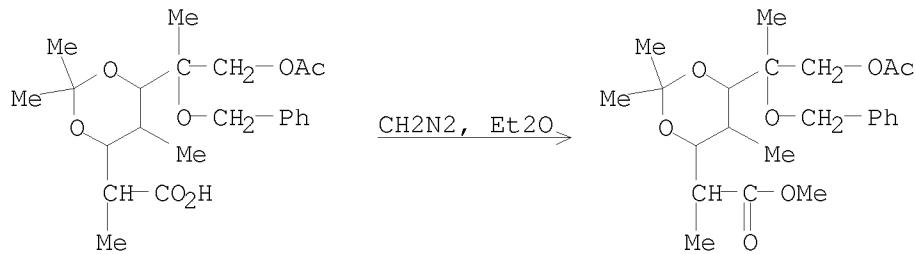


stereoisomers

REF: Journal of the Chemical Society, Chemical Communications, (5), 413-16; 1986

L2 ANSWER 23 OF 23 CASREACT COPYRIGHT 2008 ACS on STN

RX(36) OF 459



REF: Journal of Organic Chemistry, 50(12), 2095-105; 1985